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APPLICATIONS OF EXPLAINABLE ARTIFICIAL INTELLIGENCE IN PHARMACOVIGILANCE: ADVANCING PATIENT SAFETY

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ABSTRACT

Recently, a number of sectors have emphasised the need of Explainable AI (XAI), an approach that supplements the black box of artificial intelligence. Finding studies in the realm of pharmacovigilance utilising XAI is the aim of this study. Only 25 of the 781 papers that were carefully verified fit the selection requirements, despite several prior efforts to choose articles. An intuitive overview of XAI technologies' potential in pharmacovigilance is provided in this article. The included research examined drug treatment, side effects, and interaction studies based on tree models, neural network models, and graph models using clinical data, registry data, and knowledge data. Ultimately, a number of study concerns pertaining to the use of XAI in pharmacovigilance were shown to have significant obstacles. XAI is not often employed, despite the fact that artificial intelligence (AI) is actively used in patient safety and drug monitoring, collecting adverse drug response data, extracting medication-drug interactions, and forecasting effects. Thus, there should be constant discussion of the possible difficulties in using it as well as the opportunities for the future.

1. INTRODUCTION

Pharmacovigilance (PV) is defined by the World Health Organisation as the science and practices pertaining to the identification, evaluation, comprehension, and avoidance of side effects or other drug-related issues [1].

Traditional PV techniques, which may be expensive and time-consuming and can lead to adverse drug reactions (ADRs) that are not reported to medical practitioners, can be effectively supplemented by new artificial intelligence-based technologies.

Though its use in PV is still in its infancy, artificial intelligence (AI) has the potential to enhance PV. To better characterise existing pharmacological side effects and responses and to identify novel signals, a variety of machine learning (ML) approaches, together with natural language processing and data mining, may be used to electronic health records, claims databases, and social media data [2], [3].

Despite having a high predictive capability, AI-based technologies have come under fire for their incomprehensible algorithms. Explainable Artificial Intelligence (XAI) is gaining attention and study because in crucial decision-making domains like healthcare, the rationale behind a choice is just as significant as the choice itself.

By evaluating the advantages and disadvantages of current models, XAI aims to foster more trust and understanding by enhancing the transparency of AI systems and producing explanations for them [4, 5, 6]. For practitioners and consumers who are more interested in case-by-case explanations than the inner workings of a model, methods that extract information from the model's decision-making process, such post-hoc explanations, may be helpful [7].

By enabling the interpretation of decision-influencing variables, intricate internal characteristics, and learnt choice routes inside a decision process, XAI improves the explainability and transparency of AI algorithms

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[8], [9]. The potential contribution of XAI to PV monitoring was further shown by I.R. Ward et al., who used a XAI algorithm to effectively quantify the relevance of characteristics [10].

All species impacted by medical treatments should be aware of the significance of PV in medicine, and efforts to ensure medical safety must focus on strategies like medication safety reporting and the prompt and accurate sharing of information on PV activities [11]. Between 2022 and 2030, the worldwide pharmaceutical covigilance and drug safety software market is expected to develop at a compound annual growth rate (CAGR) of 10.5%, from its 2021 valuation of USD 6.9 billion (Source: www.grandviewresearch.com).

This study's objective was to evaluate the literature on XAI's use in PV by locating articles on pharmaceuticals and ML/AI, as well as the justifications for the results that were published. These research were examined from the standpoint of AI and XAI use, and the results were compiled into a summary whereby the application of XAI in the PV area is known as "PV XAI." The following highlights and discusses the primary contributions:

It is evident that this work is an early effort to examine PV studies on XAI. We discovered that, in contrast to other domains, XAI research in PV is still in its infancy and is only represented by a small number of publications and approaches.

- However, we have shown that PV XAI has good promise for medication treatment, ADRs, polypharmacies, and drug repurposing.
- Although safety concerns in actual healthcare settings could restrict the field's progress, we anticipate that PV XAI research will advance as it has in other domains, and we promote cooperation and continuous research conversations with subject-matter experts.

1.1. Purpose Of The Project

Addressing the drawbacks of black-box models, Explainable Artificial Intelligence (XAI) has become a key strategy for improving the interpretability and transparency of AI systems. Its importance is becoming more widely acknowledged in a variety of fields, including medicine. The goal of this study is to thoroughly examine how XAI is being used in pharmacovigilance, with an emphasis on enhancing patient safety.

Only 25 of the 781 relevant papers found after a thorough literature screening procedure satisfied the rigorous inclusion requirements for a thorough examination. The use of XAI approaches to pharmacovigilance tasks, including identifying adverse medication responses, evaluating drug-drug interactions, and forecasting treatment results, is intuitively summarised in this study. Clinical records, registry data, and domain knowledge were among the many data sources used in these investigations. These data sources were then processed using models including decision trees, neural networks, and graph-based frameworks.

The use of XAI is still restricted, even though AI is widely used in pharmacovigilance for tasks like monitoring and prediction. This disparity emphasises the need of greater research into interpretable models that may facilitate more open and responsible medication safety decision-making. The study's conclusion highlights the main obstacles and future directions for incorporating XAI into pharmacovigilance procedures, stressing the need for further research to fully grasp its potential to improve patient safety.

1.2. EXISTING SYSTEM

This research looked at the XAI trend in the PV industry. But the trend was also widely investigated in a wider range of areas, such as interpretable AI. They were thoroughly examined based on the same goal, despite the

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obvious distinction between Explainable AI (understanding of what various nodes represent and their significance to model performance) and Interpretable AI (capacity to ascertain cause and effect in a machine learning model).

research on XAI in drug-related applications have increased dramatically after 2019, with comparatively few research conducted between 2013 and 2018 (Fig. 1). More study on XAI in PV applications is needed, as shown by the small number of publications.

It was challenging to choose relevant search phrases for the investigation of XAI-related studies in PV; we began by hand using general keywords. Pharmacovigilance XAI (47), Pharmacovigilance "explainable artificial intelligence" (76), Pharmacovigilance explainable AI (230), Pharmacovigilance explainable ML (181), and Pharmacovigilance explainable machine learning (213), were the five search terms that were conducted. The figures in parenthesis represent the number of publications that were found using these search phrases in a Google Scholar search on June 22, 2022. A final selection of 25 unique publications was obtained after the retrieved articles were first filtered for titles and abstracts to eliminate duplicates. After that, the articles were included via a first full-text review for relevance and a second full-text review based on a selected technique.

Disadvantages

• Data complexity: In order to identify patient safety, the majority of machine learning models now in use need to be able to properly comprehend massive and complicated datasets.

• Data availability: In order to provide precise predictions, the majority of machine learning models need a lot of data. The accuracy of the model may degrade if data is not accessible in large enough amounts.

• Inaccurate labelling: The accuracy of the machine learning models that are now in use depends on how well the input dataset was used for training. Inaccurate labelling of the data prevents the model from producing reliable predictions.

1.3. PROPOSED SYSTEM

This study's objective was to evaluate the literature on XAI's use in PV by locating articles on pharmaceuticals and ML/AI, as well as the justifications for the results that were published. These research were examined from the standpoint of AI and XAI use, and the results were compiled into a summary whereby the application of XAI in the PV area is known as "PV XAI." The following highlights and discusses the primary contributions:

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- However, we have shown that PV XAI has good promise for medication treatment, ADRs, polypharmacies, and drug repurposing.
- Although safety concerns in actual healthcare settings could restrict the field's progress, we anticipate that PV XAI research will advance as it has in other domains, and we promote cooperation and continuous research conversations with subject-matter experts.

Advantages

1) We suggest Modern AI models are built on top of deep neural networks (DNNs).

2) The suggested system used tree-based algorithms, which are theoretically simple yet effective machine learning techniques that can tackle both linear and nonlinear modelling problems on both small and big datasets.

I. REQUIREMENT AND ANALYSIS

2.1. LITERATURE SURVEY

2.1.1. Overview

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"Artificial intelligence in pharmacovigilance: An overview of concepts, terminology, uses, and constraints,"
Aronson, J. K.
Artificial intelligence (AI) solutions hold great promise for improving pharmacovigilance efforts. Although they don't have to be AI specialists, pharmacovigilance professionals should be knowledgeable enough about the field to consider potential partnerships with experts. In particular, Alan Turing's study on "the imitation game" from the late 1940s and early 1950s is credited with laying the foundation for modern ideas of artificial intelligence. Today, its scope encompasses computational abilities, such as the creation of mathematical proofs; visual perception, including virtual reality and facial recognition; expert systems' decision-making; language-related skills, such as speech recognition, language processing, creative composition, and translation; and combinations of these, such as in self-driving cars. Deep structural learning may be achieved by programming machines to learn using neural networks that replicate the cognitive processes of the human brain. AI's limitations include linguistic barriers, which result from the requirement to comprehend context and interpret ambiguities, which have a special impact on translation, and database shortcomings, which need meticulous planning and curation. New methods might lead to unanticipated problems via unplanned malfunctions. Neural networks, expert systems, ontologies, natural language programming, and other forms of machine learning are examples of pertinent terminology and ideas. The use of AI techniques in pharmacovigilance has not been widely adopted. Machine learning has the potential to improve the characterisation of known adverse effects and reactions and identify new signals when combined with natural language processing and data mining to study adverse drug reactions in databases like those found in electronic health records, claims databases, and social media.
"Is artificial intelligence ready for prime time in pharmacovigilance?"
P. G. Dal and R. Ball,
The use of 'artificial intelligence' (AI) in pharmacovigilance (PV) is of considerable interest. We concentrate on the use of AI to the processing and assessment of Individual Case Safety Reports (ICSRs) submitted to the FDA Adverse Event Reporting System (FAERS), even though the US FDA is investigating the use of AI for PV in a wide sense. After describing a broad methodology for evaluating AI's preparedness for PV, we provide several instances of how AI has been used to ICSR processing and assessment in the FDA and industry. We come to the conclusion that although AI may be applied to certain elements of ICSR processing and assessment, a "human-in-the-loop" is necessary to assure high-quality performance from existing AI algorithms. A well-defined and calculable 'cognitive framework', a formal sociotechnical framework for applying AI to PV, methods for quality assurance of 'human-in-the-loop' AI systems, sizable, publicly accessible training datasets, and the creation of best practices for applying AI to PV are among the unresolved scientific and policy issues that must be resolved before the full potential of AI can be utilised for ICSR processing and evaluation. In order to facilitate widespread adoption and lay the groundwork for future development of AI approaches to other aspects of PV, practical experience with the step-by-step implementation of AI for ICSR processing and evaluation is expected to yield significant lessons.
"Comprehending, visualising, and interpreting deep learning models: Explainable Artificial Intelligence,"
K.-R. Müller, T. Wiegand, and W. Samek,

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On a growing number of challenging tasks, AI systems are performing on par with or better than humans because to the availability of big datasets and recent advancements in deep learning methods. Domains including image classification, sentiment analysis, voice recognition, and strategy gaming provide striking instances of this advancement. These very effective machine learning and artificial intelligence models, however, are often used in a black box fashion—that is, without disclosing the precise process by which they arrive at their predictions—due to their nested non-linear structure. The development of techniques for visualising, explaining, and understanding deep learning models has lately drawn more interest since this lack of transparency may be a significant disadvantage, for example, in medical applications. This essay argues for greater interpretability in artificial intelligence while summarising current advancements in the subject. Additionally, it offers two methods for elucidating deep learning model predictions: one that calculates the prediction's sensitivity to input changes, and another that meaningfully breaks down the choice in terms of the input variables. Three categorisation tasks are used to assess these approaches.

"DARPA's program for explainable artificial intelligence (XAI),"

D. Aha and D. Gunning,

A new generation of AI applications, such as those in transportation, security, medical, finance, and defence, have emerged as a result of machine learning's explosive success. These applications have enormous potential, but they are unable to adequately explain their choices and actions to human users. The goal of DARPA's explainable artificial intelligence (XAI) program is to develop AI systems whose learnt models and judgements end users can comprehend and reasonably trust. Methods for creating successful explanation interfaces, learning more explainable models, and comprehending the psychological prerequisites for persuasive explanations are all necessary to achieve this aim. By developing ML methods and concepts, tactics, and human-computer interface approaches for producing successful explanations, the XAI development teams are tackling the first two difficulties. In order to enable the XAI evaluator create an appropriate evaluation framework that the development teams will use to evaluate their systems, another XAI team is tackling the third problem by condensing, expanding, and using psychologic theories of explanation. In May 2018, the XAI teams finished the first of this four-year program. The development teams are evaluating how successfully the explanations provided by their XAM systems enhance user comprehension, user trust, and user task performance in a series of continuous assessments.

"A survey on explainable artificial intelligence,"

N. Hlupic, M. Brcic, and F. K. Došilovic,

Over the last ten years, machine learning algorithms have performed (super)humanly on a broad range of tasks thanks to the availability of massive datasets and increased processing capacity. Image recognition, audio analysis, strategic game design, and many more fields are examples of this quick progress. The lack of interpretability and openness in many state-of-the-art models is the issue. In many areas, such as healthcare and finance, where trust is based on the model's decision-making reasoning, its absence is a significant disadvantage. The scientific community is becoming interested in explainable artificial intelligence (XAI) as a result of these problems. This article provides an overview of recent advancements in supervised learning using XAI, initiates a conversation about how it relates to artificial general intelligence, and suggests future lines of inquiry.

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2.1.2 ARCHITECTURE

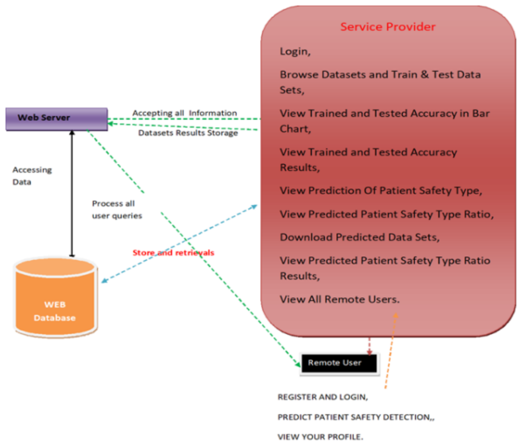

FIG.No.2.1

2.2. MODULES DESCRIPTION

2.2.1. Service Provider

The Service Provider must use a working user name and password to log in to this module. Following a successful login, he may do various tasks including browsing datasets and training and testing datasets. View Results of Trained and Tested Accuracy, View Trained and Tested Accuracy in Bar Chart, See Patient Safety Type Prediction, See Patient Safety Type Ratio Prediction, Download Predicted Data Sets, View All Remote Users and the Predicted Patient Safety Type Ratio Results.

2.2.2. View and Authorize Users

The administrator may see a list of all registered users in this module. Here, the administrator may see the user's information, like name, email, and address, and they can also grant the user permissions.

2.2.3. Remote User

A total of n users are present in this module. Before beginning any actions, the user needs register. Following registration, the user's information will be entered into the database. Following a successful registration, he must use his password and authorised user name to log in. Following a successful login, the user may do tasks including registering and logging in, predicting patient safety, and seeing their profile.

ALGORITHMS

Naïve Bayes

The supervised learning technique known as the "naive bayes approach" is predicated on the straightforward premise that the existence or lack of a certain class characteristic has no bearing on the existence or nonexistence of any other feature.

However, it seems sturdy and effective in spite of this. It performs similarly to other methods of guided learning. Numerous explanations have been put forward in the literature. We emphasise a representation bias-based explanation in this lesson. Along with logistic regression, linear discriminant analysis, and linear SVM (support vector machine), the naive bayes classifier is a linear classifier. The technique used to estimate the classifier's parameters (the learning bias) makes a difference.

Although the Naive Bayes classifier is commonly used in research, practitioners who want to get findings that are useful do not utilise it as often. On the one hand, the researchers discovered that it is very simple to build and apply, that estimating its parameters is simple, that learning occurs quickly even on extremely big datasets, and that, when compared to other methods, its accuracy is rather excellent. The end users, however, do not comprehend the value of such a strategy and do not get a model that is simple to read and implement.

As a consequence, we display the learning process's outcomes in a fresh way. Both the deployment and comprehension of the classifier are simplified. We discuss several theoretical facets of the naive bayes classifier in the first section of this lesson. Next, we use Tanagra to apply the method on a dataset. We compare the generated findings (the parameters

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of the model) to those obtained with other linear techniques such as the logistic regression, the linear discriminant analysis and the linear SVM. We see that the outcomes are quite reliable. This helps to explain why the method performs well when compared to others. We employ a variety of tools (Weka 3.6.0, R 2.9.2, Knime 2.1.1, Orange 2.0b, and RapidMiner 4.6.0) on the same dataset in the second section. We attempt above all to comprehend the produced findings.

Random Forest

Random forests, also known as random decision forests, are ensemble learning techniques that build a large number of decision trees during training for tasks like regression and classification. The class chosen by the majority of trees is the random forest's output for classification problems. The mean or average forecast of each individual tree is given back for regression tasks. The tendency of decision trees to overfit to their training set is compensated for by random decision forests. Although random forests are less accurate than gradient enhanced trees, they often perform better than choice trees. However, their performance may be impacted by data peculiarities.

Tin Kam Ho[1] developed the first algorithm for random decision forests in 1995 by using the random subspace technique, which in Ho's definition is a means of putting Eugene Kleinberg's "stochastic discrimination" approach to classification into practice.

Leo Breiman and Adele Cutler created an algorithm extension and filed for a trademark in 2006 for "Random Forests" (owned by Minitab, Inc. as of 2019).The extension builds a set of decision trees with controlled variance by combining Breiman's "bagging" concept with random feature selection, which was initially proposed by Ho[1] and then separately by Amit and Geman[13].

Businesses often employ random forests as "blackbox" models since they need minimal setup and provide accurate forecasts across a variety of inputs.

SVM

In classification problems a discriminant machine learning approach aims at discovering, based on an independent and identically distributed (iid) training dataset, a discriminant function that can accurately predict labels for newly acquired instances. Unlike generative machine learning techniques, which involve calculations of conditional probability distributions, a discriminant classification function takes a data point x and assigns it to one of the many classes that are a part of the classification job. Discriminant techniques are less effective than generative approaches, which are mostly used when prediction entails the identification of outliers. However, they need less training data and processing resources, particularly when dealing with a multidimensional feature space and when just posterior probabilities are required. Finding the equation for a multidimensional surface that optimally divides the various classes in the feature space is the geometric equivalent of learning a classifier.

SVM is a discriminant approach that, unlike genetic algorithms (GAs) or perceptrons, which are both often used for classification in machine learning, always returns the same optimum hyperplane value since it solves the convex optimisation issue analytically. The initialisation and termination criteria have a significant impact on the solutions for perceptrons. While the perceptron and GA classifier models are distinct every time training is started, training yields uniquely specified SVM model parameters for a given training set for a certain kernel that converts the data from the input space to the feature space. The only goal of

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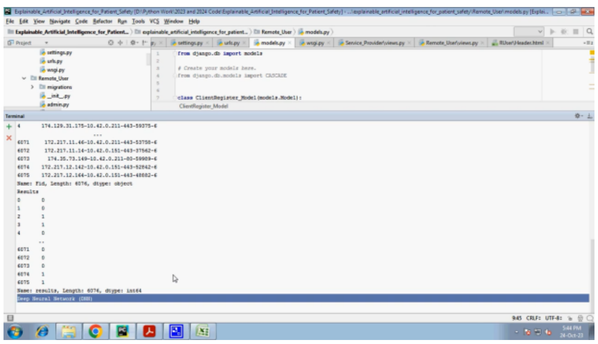
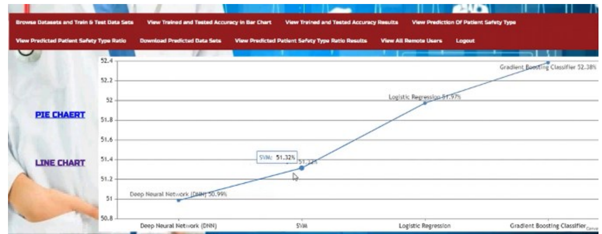
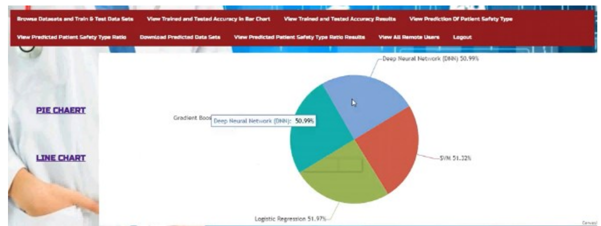
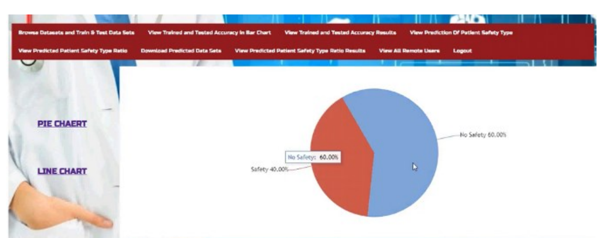
GAs and perceptrons is to reduce training error, which will result in several hyperplanes satisfying this criterion.

III. SCREEN SHOTS









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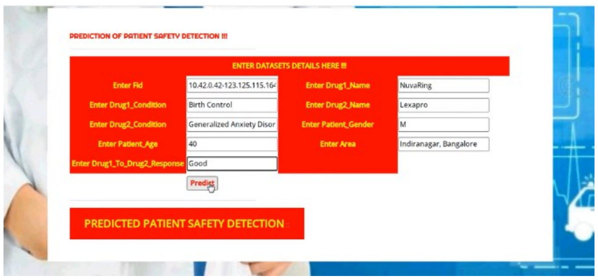

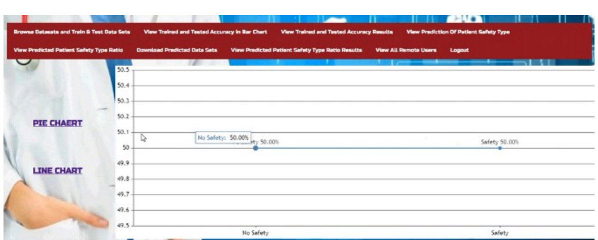

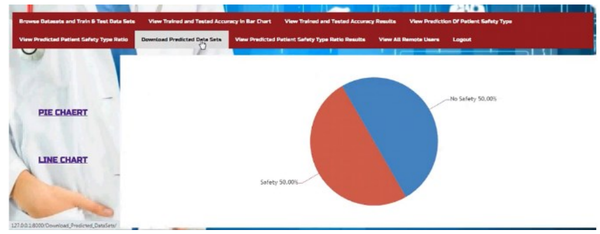

IV. CONCLUSION

In this study, we reviewed PV XAI papers and discussed recent research trends and the need for XAI research. Unlike other areas where XAI and AI are developing together, PV XAI research is still in its infancy. There are not many papers on PV XAI and the methodology is limited to a few models. However, studies are slowly beginning to show the potential of XAI research for medication monitoring and patient safety, collecting ADR and ADE information, extracting drug-drug interactions, and predicting drug treatment effects.

As in other areas, as awareness of XAI methods grows, we expect to see AI used in pharmacyovigilance and patient safety in many more ways in the coming years than those identified in this review, and the positive potential of XAI for drug therapy, ADRs and interactions is very promising. However, it is clear that the growth of this field may be limited by the lack of validated and established uses of XAI in real-world healthcare settings, and this is an area that requires further investigation. Therefore, the challenges and future prospects of XAIs in pharmacovigilance should be discussed with continued interest.

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